Localization of relativistic particles and uncertainty relations

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Localization of relativistic particles and their position-momentum uncertainty relations are not yet fully understood. We discuss two schemes of photon localization that are based on the energy density. One scheme produces a positive operator-valued measure for localization. It coincides with the number density operator and reproduces an effective 3×3 polarization density matrix. Another scheme results in a probability distribution that is conditioned on the detection. In both schemes the uncertainty relations for transversal position and momentum approach the Heisenberg bound $\Delta p \Delta z = \frac{1}{2}\hbar$.

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I. INTRODUCTION

Localized detection events provide the experimental basis of quantum field theory and quantum optics [1–3]. They are critical for understanding relativistic aspects of quantum information processing [4,5]. Nevertheless, analysis of localization in the relativistic regime [6–22] is still incomplete. A stark contrast between our ability to manipulate single photons [23,24] or trace molecules with subwavelength accuracy [25] and the lack of clarity in describing the photon localization is illustrated by a recent controversy [26,27].

One can consider localization in a space-time or on a given time slice. The solution to the former problem is given by the probability of detecting a particle during an interval of time Δt around time t in a volume ΔV around $\mathbf{x}$. If the detection time Δt can be ignored (see [28]), the problem reduces to describing localization on a time slice t. Through the paper we consider a flat space-time, use the $+---$ signature of the metric, and set $\hbar = c = 1$, unless specified otherwise. We focus on single-particle states.

The complexity of relativistic localization is highlighted by the absence of a self-adjoint time operator [29], and thus absence of space-time localization operators $\hat{X}^\mu, \mu = 0, \ldots, 3$ [9,17]. (For recent discussions see [30].) There is no unique spatial position operator, and (depending on the imposed requirements) there is no position operator for massless particles with spin larger than $\frac{1}{2}$ [8,9]. When the operator exists its components may be noncommutative, $[\hat{X}^k, \hat{X}^j] \neq 0$ [31], and the resulting probability distribution may lack a probability current or have causality problems [8,9,12–14,16].

The Newton-Wigner wave function $\psi^{\rm NW}$ [1,8] is a popular tool to describe localization of massive particles, but it is only a partial remedy [16,32]. If $|\psi^{\rm NW}(t,\mathbf{x})|^2$ is taken to be a spatial probability distribution, then there are states that violate causality [33] in the spirit of the Hegerfeldt's theorem [14] (Sec. III). In the framework of the algebraic field theory [1,2], it was shown that the localization description cannot be realized by local or quasilocal operators [17,34].

Absence of *a priori* preferable descriptions of localization motivates an operational approach. A way to substantiate the notion of particles and to reconcile it with the local quantum field theory is to analyze the (model) detectors' excitations. Investigating the space-time localization, one considers a response rate of such a detector [35–37], which leads to a Lorentz-invariant detection rate $w(t,\mathbf{x}|\rho) \equiv w(x|\rho)$, where the detection probability for a state ρ in the space-time four-volume $dtdV$ near the space-time point x is

$$dP(x,d\Omega|\rho) = w(x|\rho)dtdV. \tag{1}$$

Localization on a time slice selects a Lorentz frame that is associated with the detector(s). In this case the quantities of interest are the probability density $p(t,\mathbf{x}|\rho)$ and its current. Their interpretation as describing the evolution of the particle's position in time is not straightforward. In particular, unavoidable dark counts (response of a local detector to vacuum) that give "false positives" and a finite probability of failure, when the detectors do not "fire" even if a particle is present, should be taken into account.

In this article we focus on localizing single-particle states on a time slice. The associated probability density is constructed using three ingredients: the energy density of a quantized field, the particle's momentum-space wave function, and its energy. Two possible solutions satisfy the constraints that are imposed by quantum field theory, fulfill many of the desired properties suggested by nonrelativistic quantum mechanics, and relate to familiar objects in quantum optics. We apply these constructions to the photonic uncertainty relations and discuss possible experiments.

The rest of the paper is organized as follows. We review the general properties of localization in the next section. Section III deals with properties of energy density and two possible methods of constructing normalized probability distributions. This general theory is applied to photons in Sec. IV, and the uncertainty relations are derived in Sec. V. Section VI discusses the implications of our results, their limitations, and future directions.

II. GENERAL PROPERTIES OF LOCALIZATION

Mathematical difficulties with orthogonal projections and detection analysis led to discussion of localization in terms of positive operator-valued measures (POVMs) [16,18]. A POVM constitutes a nonorthogonal decomposition of the identity by means of positive operators $\hat{\Pi}(x)$, resulting in detection probabilities $P(x) = {\rm tr}\rho\hat{\Pi}(x)$ for the events $\{x\}$ [38,39].

In a given Minkowski frame, the sets $\Delta \subset \mathbb{R}^3$ correspond to the statements that the system is located in Δ at time t. Each set is associated with a positive operator $\hat{\Pi}(\Delta)$. The operators are not assumed to be local or quasilocal. The operators form a decomposition of identity, $\hat{\Pi}(\mathbb{R}^3) = 1$. For the disjoint sets

Δ_1 and Δ_2, the resulting operator satisfies

$$\hat{\Pi}(\Delta_1 \cup \Delta_2) = \hat{\Pi}(\Delta_1) + \hat{\Pi}(\Delta_2). \quad (2)$$

Behavior under rotations and translations is the hallmark of a position observable. Let $g \cdot \Delta = R\Delta + \mathbf{b}$ denote the action of the Euclidean group (the rotation R followed by the translation $\mathbf{b}$) on Δ and by $\hat{U}(g)$, its unitary representation. Then

$$\hat{\Pi}(g \cdot \Delta) = U(g)\hat{\Pi}(\Delta)U(g)^\dagger. \quad (3)$$

Several intuitively attractive features of position will not be realized. We do not require a sharp localizability [18]: for the disjoint Δ_1 and Δ_2 the product $\hat{\Pi}(\Delta_1)\hat{\Pi}(\Delta_2) \neq 0$. Instead of position operators $\hat{X}^l$ we have the first statistical moment operators,

$$\hat{Q}^l(t) = \int d^3\mathbf{x} x^l \hat{\Pi}(t,\mathbf{x}), \quad l = x,y,z, \quad (4)$$

where we abuse the notation by denoting the measures $\hat{\Pi}(d^3\mathbf{x})$,

$$\hat{\Pi}(\Delta) = \int_\Delta \hat{\Pi}(d^3\mathbf{x}),$$

as $\hat{\Pi}(\mathbf{x})d^3\mathbf{x}$. The operators $\hat{Q}^l$ do not commute. However, since the measurement is described by a single measure $\hat{\Pi}$, they are evaluated jointly:

$$\langle \hat{Q}^l(t) \rangle = \int d^3\mathbf{x} x^l \, p(t,\mathbf{x}), \quad p(t,\mathbf{x}) = \mathrm{tr}[\rho \hat{\Pi}(t,\mathbf{x})], \quad (5)$$

where ρ is density matrix of the system.

If the probability distribution $p(t,\mathbf{x})$ is interpreted as a time-dependent indicator of the approximate position of a particle, it is reasonable to expect the conserved current,

$$\frac{\partial p(t,\mathbf{x})}{\partial t} = -\nabla \mathbf{j}(t,\mathbf{x}), \quad (6)$$

and a causal evolution of $p(t,\mathbf{x})$. Probability density should propagate causally. Both requirements are realized below.

The localization scheme should be Lorentz covariant. However, there are different levels at which it can be realized. Consider an inhomogeneous Lorentz transformation $x \rightarrow \Lambda x + a$, where a is a four-dimensional translation and Λ some proper Lorentz transformations that connect two reference frames. For a POVM that results in the detection rate

$$w(x|\rho) = \mathrm{tr}\rho \hat{\Pi}_w(x), \quad (7)$$

the invariance of probabilities requires a unitary transformation of the POVM operators, and the state transformation law,

$$|\Psi\rangle \rightarrow \hat{U}(a,\Lambda)|\Psi\rangle, \quad (8)$$

implies [28]

$$\hat{\Pi}_w(x) \rightarrow \hat{\Pi}'_w(x') = \hat{U}(a,\Lambda)\hat{\Pi}_w(x)\hat{U}(a,\Lambda)^\dagger. \quad (9)$$

The constant time slice in one frame does not transform into a constant time slice in another frame, so no such manifest covariance can be required for $\hat{\Pi}(t,\mathbf{x})$. Instead, we expect it to be constructed in the same way in both frames, where the constituent operators transform according to their appropriate laws. The probability conservation Eq. (6) should hold true in any frame. However, there is no reason to demand that $(\rho,\mathbf{j})$ form a four-vector and transform accordingly.

III. ENERGY DENSITY AND DETECTION PROBABILITY

A. Properties

Energy density broadly agrees with our intuition of "where the particle is." Moreover, it propagates causally [32] and is directly related to photodetection [3,11,19,20]. If the electrons in a detector interact with the electric field of light, then a leading-order detection probability is proportional to the expectation value of the normal-ordered electric-field intensity operator [3], and the latter is proportional to the energy density.

In this section we discuss the resulting normalized probability distributions. We use a real scalar field for simplicity. Consider a one-particle state,

$$|\Psi\rangle = \int d\mu(p)\psi(\mathbf{p})|\mathbf{p}\rangle, \quad d\mu(p) = \frac{d^3\mathbf{p}}{(2\pi)^3 2p^0}, \quad (10)$$

where $p^0 = E_\mathbf{p} = \sqrt{m^2 + \mathbf{p}^2}$, $\langle \mathbf{p}|\mathbf{q}\rangle = (2\pi)^3(2p^0)\delta(\mathbf{p}-\mathbf{q})$, and $\int d\mu(p)|\psi|^2 = 1$. The inner product of two states is calculated in the momentum representation,

$$\langle \Psi|\Phi\rangle = \int d\mu(p)\psi^*(\mathbf{p})\phi(\mathbf{p}). \quad (11)$$

For a state $|\Psi\rangle$ the energy density equals

$$T_{00}(t,\mathbf{x}) = \langle \Psi|\hat{T}_{00}(t,\mathbf{x})|\Psi\rangle = |\nabla\psi(t,\mathbf{x})|^2 + |\partial_t\psi(t,\mathbf{x})|^2 + m^2|\psi(t,\mathbf{x})|^2, \quad (12)$$

where $\hat{T}_{00}$ is the normal-ordered Hamiltonian density, and $\psi(t,\mathbf{x})$ is the configuration space wave function (Appendix A). The energy density is positive and the Lorentz transformation properties are built into this quantity by definition.

Let us consider possible causality violations. The Hegerfeldt's theorem in its strongest version proves a superluminal speed for an exponentially localized particle. If the probability of finding it outside a sphere of radius R is bounded by

$$\mathrm{Prob}_{\notin R} < C^2 \exp(-2\gamma R), \quad (13)$$

where C is some constant and $\gamma > m$, then the state will spread faster than light. However, it was shown in [32] that no physical state can satisfy this bound. If $T_{00}(t,\mathbf{x})$ satisfies it, then both $|\psi(t,\mathbf{x})|$ and $|\partial_t\psi(t,\mathbf{x})|$ are bounded by $C\exp(-\gamma R)$. It implies that both $\psi(\mathbf{p})$ and $\psi(\mathbf{p})/E_\mathbf{p}$ are analytic functions in the strip of the complex plane that is bounded by at least $|\mathrm{Im}(\mathbf{p})| \leqslant m$, which is inconsistent with the branch cuts in $E_\mathbf{p}$ at $|\mathbf{p}| = \pm im$. Therefore the energy density cannot be "localized" enough to violate causality.

B. Normalization

If the probability to detect a particle in some volume Δ is proportional to the integral of the energy density over this volume, then the probability that a detection happened somewhere is

$$P(\mathbb{R}^3|\Psi) = K \int T_{00}(t,\mathbf{x})d^3\mathbf{x} \equiv K\langle \Psi|\hat{H}|\Psi\rangle < 1, \quad (14)$$

for some constant K. As a result, one way to obtain a probability density for the particle's position is to rescale the detection probability,

$$P^E(\Delta|\Psi) = \int \Delta \frac{T_{00}(t,\mathbf{x})}{\langle\Psi|\hat{H}|\Psi\rangle} d^3\mathbf{x}, \quad 0 \leqslant P(\Delta|\Psi) \leqslant 1. \quad (15)$$

In other words, this is a probability to find a particle in a region Δ, given that a detection occurred at all. In contrast with the POVM outcomes [4,40], this quantity is not convex [41]. Consider a state ρ which is a mixture of two pure states $|\Psi_1\rangle$ and $|\Psi_2\rangle$,

$$\rho = a\rho_1 + (1-a)\rho_2, \quad 0 < a < 1. \quad (16)$$

According to Eq. (15), probability densities for the states $\rho_i = |\Psi_i\rangle\langle\Psi_i|$ are

$$p_i^E(t,\mathbf{x}) = \frac{\mathrm{tr}\,\rho_i \hat{T}_{00}(t,\mathbf{x})}{\mathrm{tr}\,\rho_i \hat{H}}. \quad (17)$$

By using either the above definition or the convexity property we reach

$$p_\rho^E(t,\mathbf{x}) = \frac{\mathrm{tr}\,\rho \hat{T}_{00}(t,\mathbf{x})}{\mathrm{tr}\,\rho \hat{H}} \neq \frac{a\mathrm{tr}\,\rho_1 \hat{T}_{00}(t,\mathbf{x}) + (1-a)\mathrm{tr}\,\rho_2 \hat{T}_{00}(t,\mathbf{x})}{a\mathrm{tr}\,\rho_1 \hat{H} + (1-a)\mathrm{tr}\,\rho_2 \hat{H}}, \quad (18)$$

and these two expressions are generally different. This behavior is typical for postselected quantities [42].

Linearity is restored if normalization of the probability distribution follows the operator-valued measure. We construct a POVM element as

$$\hat{\Pi}(t,\mathbf{x}) = \hat{H}^{-1/2}\hat{T}_{00}(t,\mathbf{x})\hat{H}^{-1/2}. \quad (19)$$

The action of $\hat{H}^{-1}$ is is well defined when we restrict it to the nonvacuum states. It was shown in [21] that the Born-Infeld position operator [7] that is obtained from the first moment of the energy distribution $\hat{\mathbf{N}} = \int d^3\mathbf{x}\,\mathbf{x}\hat{T}_{00}$ equals the first moment of this operator density,

$$\frac{1}{2}(\hat{H}^{-1}\hat{\mathbf{N}} + \hat{\mathbf{N}}\hat{H}^{-1}) = \int d^3\mathbf{x}\,\mathbf{x}\hat{\Pi}(t,\mathbf{x}). \quad (20)$$

The probability density $\langle\Psi|\hat{\Pi}(t,\mathbf{x})|\Psi\rangle$ can be written as the energy density of a classical field,

$$p(t,\mathbf{x}) := \langle\Psi|\hat{\Pi}(t,\mathbf{x})|\Psi\rangle = [|\nabla\tilde{\psi}(t,\mathbf{x})|^2 + |\partial_t\tilde{\psi}(t,\mathbf{x})|^2 + m^2|\tilde{\psi}(t,\mathbf{x})|^2], \quad (21)$$

where the additional $E_\mathbf{p}^{-1/2}$ factor is added to $\psi(\mathbf{p})$,

$$\tilde{\psi}(t,\mathbf{x}) = \int d\mu(p)\frac{\tilde{\psi}}{\sqrt{E_\mathbf{p}}}(\mathbf{p})e^{i(\mathbf{p}\cdot\mathbf{x}-Et)}. \quad (22)$$

The probability current $j^l(t,\mathbf{x}) = \langle\hat{T}^{0l}\rangle$ is obtained similarly (Appendix A). Working in the momentum space representation, it is easy to see that indeed,

$$p \geqslant 0, \quad \int p(t,\mathbf{x})d^3\mathbf{x} = 1, \quad \dot{p} = -\nabla\cdot\mathbf{j}, \quad (23)$$

where the energy-momentum conservation $\partial_\mu\hat{T}^{0\mu} = 0$ results in the continuity equation for the probability density.

The arguments of [32] for the energy density are equally well applied to our probability distribution p, so Hegerfeldt's theorem does not present a paradox. We note that the presence of the Hamiltonian makes $\hat{\Pi}$ a nonlocal operator, in agrement with [17,34]. A nonrelativistic limit is obtained by expanding $p(t,\mathbf{x})$ in powers of $\mathbf{p}/m$ (Appendix A).

IV. LOCALIZATION OF PHOTONS

Following [21,26] we use the Riemann-Silberstein vector

$$\mathbf{F} := \mathbf{E} + i\mathbf{B}. \quad (24)$$

The classical energy density in a free space is then

$$T_{00} = \tfrac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2) = \tfrac{1}{2}\mathbf{F}^*\cdot\mathbf{F}. \quad (25)$$

We work in the radiation gauge (so $\mathbf{E} = -\dot{\mathbf{A}}$ and $\mathbf{B} = \nabla\times\mathbf{A}$) and write the solutions of the wave equation with the help of right and left polarization vectors $\boldsymbol{\epsilon}_\mathbf{p}^\pm$,

$$\mathbf{p}\times\boldsymbol{\epsilon}_\mathbf{p}^\pm = \mp i|\mathbf{p}|\boldsymbol{\epsilon}_\mathbf{p}^\pm, \quad (26)$$

that satisfy the convention

$$\boldsymbol{\epsilon}_\mathbf{p} := \boldsymbol{\epsilon}_\mathbf{p}^+ = \boldsymbol{\epsilon}_\mathbf{p}^{-*} = \boldsymbol{\epsilon}_{-\mathbf{p}}^*, \quad \boldsymbol{\epsilon}_\mathbf{p}^*\cdot\boldsymbol{\epsilon}_\mathbf{p} = 1, \quad \boldsymbol{\epsilon}_\mathbf{p}^2 = 0. \quad (27)$$

We adapt Wigner's construction of the massless representation of the Poincaré group to the construction of the polarization basis vectors $\boldsymbol{\epsilon}_\mathbf{p}^\pm$ [4,44]. For $\mathbf{p} = p(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$,

$$\boldsymbol{\epsilon}_\mathbf{p} = \tfrac{1}{\sqrt{2}}(\cos\theta\cos\varphi - i\sin\varphi, \cos\theta\sin\varphi + i\cos\varphi, -\sin\theta). \quad (28)$$

Writing the quantum field as

$$\hat{\mathbf{A}}(t,\mathbf{x}) = \int d\mu(p)\sum_{\lambda=\pm1}\left(\boldsymbol{\epsilon}_\mathbf{p}^\lambda\alpha_{\mathbf{p}\lambda}e^{-ip\cdot x} + \boldsymbol{\epsilon}_\mathbf{p}^{\lambda*}\alpha_{\mathbf{p}\lambda}^\dagger e^{ip\cdot x}\right), \quad (29)$$

we obtain the standard commutation relations (Appendix B), and the Riemann-Silberstein operator,

$$\hat{\mathbf{F}} = \hat{\mathbf{E}} + i\hat{\mathbf{B}} = 2i\int d\mu(p)E_\mathbf{p}\boldsymbol{\epsilon}_\mathbf{p} \times (\alpha_{\mathbf{p}+}e^{-ip\cdot x/\hbar} + \alpha_{\mathbf{p}-}^\dagger e^{ip\cdot x/\hbar}). \quad (30)$$

Energy density then becomes

$$\hat{T}_{00} = \frac{1}{2}::\hat{\mathbf{F}}^\dagger\cdot\hat{\mathbf{F}}:: = 2\sum_{\lambda=\pm1}\int d\mu(p)d\mu(q)E_\mathbf{p}E_\mathbf{q}\,\boldsymbol{\epsilon}_\mathbf{p}^*\cdot\boldsymbol{\epsilon}_\mathbf{q} \times \alpha_{\mathbf{p}\lambda}^\dagger\alpha_{\mathbf{q}\lambda}e^{i(p-q)\cdot x/\hbar}, \quad (31)$$

where the terms that annihilate one-particle states are dropped. A straightforward calculation leads to a POVM,

$$\hat{\Pi}(t,\mathbf{x}) = \hat{H}^{-1/2}\hat{T}_{00}(t,\mathbf{x})\hat{H}^{-1/2} = 2\sum_{\lambda=\pm1}\int d\mu(p)d\mu(q)\sqrt{E_\mathbf{p}E_\mathbf{q}}\boldsymbol{\epsilon}_\mathbf{p}^*\cdot\boldsymbol{\epsilon}_\mathbf{q} \times \alpha_{\mathbf{p}\lambda}^\dagger\alpha_{\mathbf{q}\lambda}e^{i(p-q)\cdot x/\hbar}. \quad (32)$$

For a generic one-photon state

$$|\Psi\rangle = \sum_{\lambda=\pm1}\int d\mu(p)\psi_\lambda(\mathbf{p})a_{\mathbf{p}\lambda}^\dagger|0\rangle, \quad (33)$$

the energy density can be compactly written with the three-vector wave function [3]

$$\boldsymbol{\phi}_\lambda(t,\mathbf{x}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{p}\boldsymbol{\epsilon}^\lambda_\mathbf{p}\psi_\lambda(\mathbf{p})e^{-ip\cdot x/\hbar}, \tag{34}$$

as

$$T_{00}(x) = \langle\Psi|\hat{T}_{00}(x)|\Psi\rangle = \frac{1}{2}\sum_{\lambda=\pm1}|\boldsymbol{\phi}_\lambda(x)|^2. \tag{35}$$

On the other hand, the probability density is given by the Newton-Wigner wave function,

$$p(t,\mathbf{x}) = \langle\Psi|\hat{\Pi}(t,\mathbf{x})|\Psi\rangle = \sum_{\lambda=\pm1}|\mathbf{f}_\lambda(t,\mathbf{x})|^2, \tag{36}$$

where

$$\mathbf{f}_\lambda(t,\mathbf{x}) = \int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathbf{f}_\lambda(\mathbf{p})e^{-ip\cdot x/\hbar} = \int\frac{d^3\mathbf{p}}{(2\pi)^3}\boldsymbol{\epsilon}^\lambda_\mathbf{p}\frac{\psi_\lambda(\mathbf{p})}{\sqrt{2E_\mathbf{p}}}e^{-ip\cdot x/\hbar}. \tag{37}$$

Several observations are in order. The configuration space wave function has the Newton-Wigner form (see, e.g., [43]), even if it is not an eigenfunction of the position operator. The POVM $\hat{\Pi}$ is identical with Mandel's number density operator [10]. The two wave functions are related as

$$\boldsymbol{\phi}_\lambda(\mathbf{p}) = \sqrt{2E_\mathbf{p}}\,\mathbf{f}_\lambda(\mathbf{p}). \tag{38}$$

The effective polarization density matrix was introduced on the formal grounds [4,44] as an analog of the 3×3 classical correlation matrix [3]. It results in the probabilities $P_a(\rho) = \operatorname{tr}\Pi_a\rho$ for a class of POVMs $\{\Pi_a\}$ that are based on a simple photodetection model [45]. This density matrix is given by [4,45]

$$\rho_{mn} = \int d\mu(p)\sum_{\lambda,\lambda'=\pm1}\psi_\lambda(\mathbf{p})\psi_{\lambda'}(\mathbf{p})^*\left(\boldsymbol{\epsilon}^\lambda_\mathbf{p}\right)_m\left(\boldsymbol{\epsilon}^{\lambda'}_\mathbf{p}\right)^*_n. \tag{39}$$

Introducing the vectorial components of the wave function as $f_m = (\mathbf{f}_+)_m + (\mathbf{f}_-)_m$, we see from Eq. (37) that

$$\rho_{mn} = \int\frac{d^3\mathbf{p}}{(2\pi)^3}f_m(\mathbf{p})f_n(\mathbf{p})^* = \int d^3\mathbf{x}f_m(t,\mathbf{x})f_n(t,\mathbf{x})^*, \tag{40}$$

again, similarly to the nonrelativistic quantum mechanics.

V. UNCERTAINTY RELATIONS

The uncertainty relations that involve the position operator were analyzed by Bialynicki-Birula and Bialynicka-Birula in [26]. Here instead we consider the statistics derived from the probability density of Eq. (36) and show that the variances saturate the Heisenberg bound $\Delta q\Delta p \geqslant \hbar/2$. Consider a one-photon state with Gaussian profiles in both x (the average propagation direction) and the transversal (y and z) components of the momentum, which is built as a superposition of the right-polarized components only:

$$f(\mathbf{p}) = \frac{\psi_+(\mathbf{p})}{\sqrt{2E_\mathbf{p}}} = \frac{2\pi^{3/4}w}{\sqrt{\sigma}}\exp\left(-\frac{w^2\left(p_y^2+p_z^2\right)}{4}\right) \times\exp\left(-\frac{(p_x-p_0)^2}{2\sigma^2}\right). \tag{41}$$

For a classical beam w is the radius at which the intensity falls off to $1/2e^2$ of its maximum value on the axis of symmetry [3,25], and we take $1/w,\sigma \ll p_0$. Having in mind the actual experimental setups, we consider the transversal uncertainty relations.

The momentum space wave function has the standard probabilistic interpretation, i.e., for any power k,

$$\left\langle p_l^k\right\rangle = \int d\mu(p)p_l^k|\psi_+(\mathbf{p})|^2 = \int d^3\mathbf{p}\, p_l^k|f(\mathbf{p})|^2, \tag{42}$$

where $l = x,y,z$. The first moments are $\langle p_y\rangle = \langle p_z\rangle = 0$, $\langle p_x\rangle = p_0$, and the second moments of the transversal momentum are

$$\left\langle p_y^2\right\rangle = \left\langle p_z^2\right\rangle = 1/w^2. \tag{43}$$

We expand the polarization vector $\boldsymbol{\epsilon}_\mathbf{p}$ in Eq. (37) in the inverse powers of p_0 and perform the Gaussian integrations, obtaining

$$p(t,\mathbf{x}) = p_0(t,\mathbf{x})\left(1+\frac{4(y^2+z^2)-2w^2}{p_0^2w^4}+O\left(p_0^{-4}\right)\right), \tag{44}$$

where $p_0(t,\mathbf{x}) = |f(t,\mathbf{x})|^2$ is the scalar Gaussian probability density. As a result, in $\langle y\rangle = \langle z\rangle = 0$ and

$$\langle z^2\rangle = \langle y^2\rangle = \frac{w^2}{4}+\frac{1}{2p_0^2}+O\left(p_0^{-4}\right), \tag{45}$$

approaching the usual nonrelativistic bound,

$$\Delta z\Delta p_z \geqslant \frac{\hbar}{2}\left(1+\frac{\hbar^2}{p_0^2w^2}+O\left(p_0^{-4}\right)\right), \tag{46}$$

with the identical expression for the y component, and we restored the use of $\hbar$.

Interpretation of $\mathbf{f}_\lambda(t,\mathbf{x})$ as the position probability amplitude faces a difficulty when contrasted with the detection probability of Eq. (14). Because of Eq. (38) the photon that is "localized" in a bounded region Δ (i.e., $\mathbf{f}_\lambda(t,\mathbf{x}) = 0$ for $\mathbf{x}\in\mathbb{R}^3\setminus\Delta$) has a nonzero detection probability outside it [3,11]. Therefore it is useful to estimate the uncertainty using the normalized counting statistics that is represented by

$$p^E(t,\mathbf{x}) = \frac{|\boldsymbol{\phi}_+(t,\mathbf{x})|^2+|\boldsymbol{\phi}_-(t,\mathbf{x})|^2}{2E}, \tag{47}$$

where the expectation of energy is

$$E = \frac{1}{2}\int d^3\mathbf{x}[|\boldsymbol{\phi}_+(t,\mathbf{x})|^2+|\boldsymbol{\phi}_-(t,\mathbf{x})|^2]. \tag{48}$$

Expanding

$$\sqrt{E_\mathbf{p}} = \left([p_0+(p_x-p_0)]^2+p_y^2+p_z^2\right)^{1/4} \tag{49}$$

in the inverse powers of the momentum p_0 allows one to obtain the series expansion of $\boldsymbol{\phi}(t,\mathbf{x})$ and E. Statistical moments can be obtained either from the resulting probability density p^E or by the techniques of Appendix A. The uncertainty for the state ψ_+ of Eq. (41) becomes

$$\langle y^2\rangle_E = \langle z^2\rangle_E = \frac{1}{4}\left(w^2+\frac{1}{p_0^2}+O\left(p_0^{-4}\right)\right) = \frac{1}{4}\left(w^2+\frac{\lambda_0^2}{4\pi^2}+O\left(\lambda_0^4\right)\right), \tag{50}$$

where $\lambda_0 = h/p_0$ is the peak wavelength. Transversal momentum measurements are performed with he same detectors that are positioned behind a suitably arranged lens system [23,46]. The latter implements the Fourier transform between $\boldsymbol{\phi}(\mathbf{x})$ and $\boldsymbol{\phi}(\mathbf{p})$. Using $\boldsymbol{\phi}(\mathbf{p})$ to calculate the statistical moments leads to

$$\langle p_z^2\rangle_E = \langle p_y^2\rangle_E = \frac{1}{w^2}\left(1 + \frac{1}{p_0^2 w^2} + O\left(p_0^{-4}\right)\right) = \frac{1}{w^2}\left(1 + \frac{\lambda_0^2}{4\pi^2 w^2} + O\left(\lambda_0^4\right)\right). \quad (51)$$

VI. DISCUSSION

Within the domain of validly of a single-particle picture, the energy density provides a satisfactory description of localization. By dropping the insistence on local operators, we not only conform to the general results of the quantum field theory, but break a vicious cycle where the only operator that satisfies all the "reasonable" requirements of localization is identically zero.

For photons the resulting POVM $\hat{\Pi}(t,\mathbf{x})$ coincides with the photon density operator. The resulting probability density shows a curious property: it is given by the absolute value squared of the configuration space wave function of the Newton-Wigner form, even if the Newton-Wigner position operator for photons does not exist. The effective density matrix is a necessary mode of polarization description if the wave packet spread is important. Our scheme provides a direct link between the momentum space and configuration space descriptions of polarization.

We can settle the controversy about the photon uncertainty relations. Our scheme results in the expressions for probability density that are identical with that of [26], but by accepting the standard definitions of the statistical analysis approach the nonrelativistic Heisenberg bound $\Delta q \Delta p = \hbar/2$. It is remains to be seen how close it is possible to reach this limit by optimizing the state ψ.

The one-particle picture has a limited validity. Particles cannot be confined into a volume with a typical dimension smaller than

$$\sqrt[3]{\Delta} > \frac{1}{\langle E\rangle}, \quad (52)$$

where $\langle E\rangle$ is the particle's expected energy [6]. The very concept of particles takes a somewhat "nebulous character" [35] in field theories in a curved space-time or for accelerated observers. A simple example of when this construction is not applicable is the Unruh effect [36]. An accelerated detector that moves in the Minkowski vacuum responds as an inertial detector would if immersed into a thermal bath of temperature

$$T = a/(2\pi k_B), \quad (53)$$

where k_B is Boltzmann's constant and a the proper acceleration. However, the expectation of the renormalized stress-energy tensor is zero in both inertial and accelerated frames.

In more complicated settings the question of positivity becomes acute. Classical energy density is always positive, which is to say that the stress-energy tensor for the scalar field satisfies the weak energy condition (WEC) $T_{\mu\nu}u^\mu u^\nu \geqslant 0$, where u^μ is a causal vector. In quantum field theory [1,2] it is impossible. There are states $|\Upsilon\rangle$ that violate WEC, namely, $\langle\Upsilon|T_{\mu\nu}u^\mu u^\nu|\Upsilon\rangle \leqslant 0$ holds [47], where $T_{\mu\nu}$ now is a renormalized stress energy operator. For example, squeezed states of electromagnetic [3] or scalar field have negative energy densities [48–50]. It is known that even if WEC is violated the average WEC still holds when the averaging is done over the world line of a geodesic observer (inertial observer in the Minkowski space-time) [51]. There are also more stringent quantum inequalities that limit the amount of the WEC violation. Instead of an infinite time interval they deal with a sampling that is described by a function with a typical width t_0 [50]. The behavior of fields subjected to boundary conditions is more complicated, but similar constraints exist also in these cases [50]. To meet our ends we need the analogous inequalities to hold for a spatial averaging. This is, however, impossible. A class of quantum states was constructed for a massless, minimally coupled free scalar field (superposition of the vacuum and multimode two-particle states). These states can produce an arbitrarily large amount of negative energy in a given finite region of space at a fixed time [52]. In this and similar cases, the spatial averaging over part of a constant time surface does not produce a positive quantity. An interesting line of research is to trace the emergence of well-defined particles in these complicated situations.

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APPENDIX A: REAL SCALAR FIELD

We adapt the following normalization convention for the sates and operators:

$$|\mathbf{p}\rangle = \alpha_{\mathbf{p}}^\dagger|0\rangle, \quad [\alpha_{\mathbf{q}},\alpha_{\mathbf{p}}^\dagger] = (2\pi)^3(2E_{\mathbf{p}})\delta^{(3)}(\mathbf{q}-\mathbf{p}), \quad (A1)$$

so the scalar field is written as

$$\hat{\phi} = \int d\mu(p)(\alpha_{\mathbf{p}}e^{-ip\cdot x} + \alpha_{\mathbf{p}}^\dagger e^{ip\cdot x}). \quad (A2)$$

For a one-particle state of Eq. (10), its wave function in the configuration space is defined by a generalized Fourier transform as

$$\psi(\mathbf{x},t) = \int d\mu(p)\psi(\mathbf{p})e^{i(\mathbf{p}\cdot\mathbf{x}-Et)}. \quad (A3)$$

The normal-ordered energy density is

$$\hat{T}_{00}(t,\mathbf{x}) = ::\mathcal{H}(t,\mathbf{x}):: = \frac{1}{2}\int d\mu(p)d\mu(q)(E_{\mathbf{p}}E_{\mathbf{q}} + \mathbf{p}\cdot\mathbf{q} + m^2) \times (\alpha_{\mathbf{p}}^\dagger\alpha_{\mathbf{q}}e^{i(p-q)\cdot x} + \alpha_{\mathbf{q}}^\dagger\alpha_{\mathbf{p}}e^{-i(p-q)\cdot x}) + \cdots = \int d\mu(p)d\mu(q)(E_{\mathbf{p}}E_{\mathbf{q}} + \mathbf{p}\cdot\mathbf{q} + m^2)\alpha_{\mathbf{p}}^\dagger\alpha_{\mathbf{q}}e^{i(p-q)\cdot x}, \quad (A4)$$

where ... terms have zero matrix elements between the states with the same definite number of particles. Similarly, the normal-ordered momentum density is

$$\hat{T}_{0k}(t,\mathbf{x}) = ::\frac{\partial\hat{\phi}}{\partial x^0}\frac{\partial\hat{\phi}}{\partial x^k}:: = \int d\mu(p)d\mu(q)E_{\mathbf{p}}q_k \times (\alpha^\dagger_{\mathbf{p}}\alpha_{\mathbf{q}}e^{i(p-q)\cdot x} + \alpha^\dagger_{\mathbf{q}}\alpha_{\mathbf{p}}e^{-i(p-q)\cdot x}) + \cdots. \quad \text{(A5)}$$

The expectation values are

$$\langle\Psi|\hat{T}_{00}|\Psi\rangle = \int d\mu(k)d\mu(k')(E_{\mathbf{k}}E_{\mathbf{k}'} + \mathbf{k}\cdot\mathbf{k}' + m^2) \times \psi^*(\mathbf{k})\psi(\mathbf{k}')e^{i(k-k')\cdot x} = |\nabla\psi(t,\mathbf{x})|^2 + |\partial_t\psi(t,\mathbf{x})|^2 + m^2|\psi(t,\mathbf{x})|^2 \quad \text{(A6)}$$

and

$$\langle\Psi|\hat{T}_{0j}|\Psi\rangle = -2\int d\mu(k)d\mu(k')E_{\mathbf{k}}k_j\psi^*(\mathbf{k})\psi(\mathbf{k}')e^{i(k-k')\cdot x}, \quad \text{(A7)}$$

respectively. Hence the Hamiltonian and its inverse square root are given by

$$\hat{H} = \int \hat{T}_{00}dV = \int d\mu(p)E_{\mathbf{p}}\alpha^\dagger_{\mathbf{p}}\alpha_{\mathbf{p}}, \qquad \hat{H}^{-1/2} = \int d\mu(p), \quad \frac{1}{\sqrt{E_{\mathbf{p}}}}\alpha^\dagger_{\mathbf{p}}\alpha_{\mathbf{p}}, \quad \text{(A8)}$$

respectively, and the POVM element $\hat{\Pi}$ is given by

$$\hat{\Pi}(t,\mathbf{x}) = \hat{H}^{-1/2}\hat{T}_{00}(t,\mathbf{x})\hat{H}^{-1/2} = \int d\mu(p)d\mu(q)\frac{1}{\sqrt{E_{\mathbf{p}}E_{\mathbf{q}}}} \times (E_{\mathbf{p}}E_{\mathbf{q}} + \mathbf{p}\cdot\mathbf{q} + m^2)\alpha^\dagger_{\mathbf{p}}\alpha_{\mathbf{q}}e^{i(p-q)\cdot x}. \quad \text{(A9)}$$

This results in the following probability density:

$$p(t,\mathbf{x}) = \langle\Psi|\hat{\Pi}(t,\mathbf{x})|\Psi\rangle = \int d\mu(k)d\mu(k')\frac{1}{\sqrt{E_{\mathbf{k}}E_{\mathbf{k}'}}} \times (E_{\mathbf{k}}E_{\mathbf{k}'} + \mathbf{k}\cdot\mathbf{k}' + m^2)\psi^*(\mathbf{k})\psi(\mathbf{k}')e^{i(k-k')\cdot x} = |\nabla\tilde{\psi}(t,\mathbf{x})|^2 + |\partial_t\tilde{\psi}(t,\mathbf{x})|^2 + m^2|\tilde{\psi}(t,\mathbf{x})|^2. \quad \text{(A10)}$$

Similarly, the probability current is

$$\hat{j}_l(t,x) = \hat{H}^{-1/2}\hat{T}_{0l}(t,\mathbf{x})\hat{H}^{-1/2}. \quad \text{(A11)}$$

Introducing

$$f(\mathbf{p},\mathbf{q}) := \frac{1}{4E_{\mathbf{p}}^{3/2}E_{\mathbf{q}}^{3/2}}(E_{\mathbf{p}}E_{\mathbf{q}} + \mathbf{p}\cdot\mathbf{q} + m^2), \quad \text{(A12)}$$

we express the expectation of $\mathbf{x}$ at time $t = 0$ as

$$\langle\mathbf{x}(0)\rangle = -i\int d^3\mathbf{x}\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i(p-q)\cdot x}\nabla_{\mathbf{p}} \times [f(\mathbf{p},\mathbf{q})\psi^*(\mathbf{p})\psi(\mathbf{q})] \quad \text{(A13)}$$

and the second moment as

$$\langle x_l^2(0)\rangle = \int d^3\mathbf{x}\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i(p-q)\cdot x}\partial_{p_l}\partial_{q_l} \times [f(\mathbf{p},\mathbf{q})\psi^*(\mathbf{p})\psi(\mathbf{q})]. \quad \text{(A14)}$$

These may be more conveniently expressed as

$$\langle\mathbf{x}\rangle = i\int\frac{d^3\mathbf{p}}{(2\pi)^3}\left(\frac{\mathbf{p}}{4E_{\mathbf{p}}^3}|\psi(\mathbf{p})|^2 - \frac{1}{2E_{\mathbf{p}}}\psi(\mathbf{p})\nabla_{\mathbf{p}}\psi(\mathbf{p})^*\right) \quad \text{(A15)}$$

and

$$\langle x_l^2\rangle = \int\frac{d^3\mathbf{p}}{(2\pi)^3}\left(\frac{2E_{\mathbf{p}}^2 - p_l^2}{8E_{\mathbf{p}}^5}|\psi(\mathbf{p})|^2 - \frac{p_l}{2E_{\mathbf{p}}^3}\partial_{p_l}|\psi(\mathbf{p})|^2 + \frac{1}{2E_{\mathbf{p}}}|\partial_{p_l}\psi(\mathbf{p})|^2\right). \quad \text{(A16)}$$

For $t \neq 0$ we make the substitution

$$i\frac{\partial f}{\partial p_k} \to \left(-\frac{\partial E_{\mathbf{p}}}{\partial p_k}t + i\frac{\partial}{\partial p_k}\right)f, \quad \text{(A17)}$$

hence, e.g.,

$$\langle\mathbf{x}(t)\rangle = -i\int d^3\mathbf{x}\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i(p-q)\cdot x}\nabla_{\mathbf{p}}[f(\mathbf{p},\mathbf{q})\psi^*(\mathbf{p})\psi(\mathbf{q})] + t\int\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{\mathbf{p}}{E_{\mathbf{p}}}f(\mathbf{p},\mathbf{p})\psi^*(\mathbf{p})\psi(\mathbf{p}) = \langle\mathbf{x}(t=0)\rangle + \langle\mathbf{v}\rangle t. \quad \text{(A18)}$$

To obtain the nonrelativistic identification of a wave function we expand Eq. (A10) in powers of $\mathbf{p}/m$, and find that the leading term agrees with the following nonrelativistic value:

$$\lim_{|\mathbf{p}|\ll m}\psi(\mathbf{p})/\sqrt{2m} = \psi(\mathbf{p})^{\text{nonrel}}. \quad \text{(A19)}$$

APPENDIX B: ELECTROMAGNETIC FIELD

In the section we restore the factors $\hbar$ and c. The classical gauge-invariant Lagrangian is

$$\mathcal{L} = \tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}, \quad \text{(B1)}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic tensor. We quantize the canonical variables $\mathbf{A}$ (configuration variables) and $-\mathbf{E}$ (momenta) in the radiation gauge. The creation and annihilation operators satisfy

$$[\alpha_{\mathbf{p}\lambda},\alpha^\dagger_{\mathbf{q}\lambda'}] = (2\pi)^3(2E_{\mathbf{p}})\delta_{\lambda\lambda'}\delta^{(3)}(\mathbf{q}-\mathbf{p}). \quad \text{(B2)}$$

Hence

$$\hat{\mathbf{A}}(t,\mathbf{x}) = \frac{c}{\sqrt{\hbar}}\int d\mu(p)\sum_{\lambda=\pm1}\left(\boldsymbol{\epsilon}^\lambda_{\mathbf{p}}\alpha_{\mathbf{p}\lambda}e^{-ip\cdot x/\hbar} + \boldsymbol{\epsilon}^{\lambda*}_{\mathbf{p}}\alpha^\dagger_{\mathbf{p}\lambda}e^{ip\cdot x/\hbar}\right), \qquad d\mu(p) = \frac{1}{(2\pi)^3}\frac{d^3\mathbf{p}}{(2E_{\mathbf{p}})}, \quad \text{(B3)}$$

and the field commutation relations are

$$[\hat{A}^m(t,\mathbf{x}),\hat{E}^n(t,\mathbf{y})] = -i\hbar c\delta^{mn}\delta^{(3)}(\mathbf{x}-\mathbf{y}), \qquad [\hat{B}_k(t,\mathbf{x}),\hat{E}_l(t,\mathbf{y})] = i\hbar c\,\varepsilon_{klm}\partial_{x^m}\delta^{(3)}(\mathbf{x}-\mathbf{y}), \quad \text{(B4)}$$

where ε_{klm} is the totally antisymmetric symbol.

Energy density takes the form

$$\hat{T}_{00} = \frac{1}{2} :: \hat{\mathbf{F}}^{\dagger} \cdot \hat{\mathbf{F}} :: = \frac{2}{\hbar^3} \int d\mu(p) d\mu(q) E_{\mathbf{p}} E_{\mathbf{q}}\, \boldsymbol{\epsilon}^{*}_{\mathbf{p}} \cdot \boldsymbol{\epsilon}_{\mathbf{q}} \times (\alpha^{\dagger}_{\mathbf{p}+} \alpha_{\mathbf{q}+} e^{i(p-q)\cdot x/\hbar} + \alpha^{\dagger}_{\mathbf{q}-} \alpha_{\mathbf{p}-} e^{-i(p-q)\cdot x/\hbar}), \quad \text{(B5)}$$

where the terms that annihilate states with a fixed number of particles are dropped.

Similarly, momentum density is

$$\hat{T}_{0k}/c = \frac{1}{2ic} :: \hat{\mathbf{F}}^{\dagger} \times \hat{\mathbf{F}} :: = \frac{2}{\hbar^3 c} \int d\mu(p) d\mu(q) E_{\mathbf{p}} E_{\mathbf{q}}\, \boldsymbol{\epsilon}^{*}_{\mathbf{p}} \times \boldsymbol{\epsilon}_{\mathbf{q}} (\alpha^{\dagger}_{\mathbf{p}+} \alpha_{\mathbf{q}+} e^{i(p-q)\cdot x/\hbar} + \alpha^{\dagger}_{\mathbf{q}-} \alpha_{\mathbf{p}-} e^{-i(p-q)\cdot x/\hbar}) \quad \text{(B6)}$$

and the Hamiltonian is

$$\hat{H} = \int d\mu(p) E_{\mathbf{p}} \sum_{\lambda=\pm 1} \alpha^{\dagger}_{\mathbf{p}\lambda} \alpha_{\mathbf{p}\lambda}. \quad \text{(B7)}$$

The probability density $p(t,\mathbf{x}) = \langle \Psi \hat{\Pi}(t,\mathbf{x}) | \Psi \rangle$ equals

$$p(t,\mathbf{x}) = \frac{2}{\hbar^3} \int d\mu(k) d\mu(k') \sqrt{E_{\mathbf{k}} E_{\mathbf{k}'}}\, [\boldsymbol{\epsilon}^{*}_{\mathbf{k}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}'} \psi^{*}_{+}(\mathbf{k}) \psi_{+}(\mathbf{k}') + \boldsymbol{\epsilon}_{\mathbf{k}} \cdot \boldsymbol{\epsilon}^{*}_{\mathbf{k}'} \psi^{*}_{-}(\mathbf{k}) \psi_{-}(\mathbf{k}')] e^{i(k-k')\cdot x/\hbar}. \quad \text{(B8)}$$

Similarly, the probability current is given by

$$\hat{j}_m(t,\mathbf{x}) = \langle \Psi | \hat{H}^{-1/2} \hat{T}_{0m}(t,\mathbf{x}) \hat{H}^{-1/2} | \Psi \rangle / c. \quad \text{(B9)}$$

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